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Thermodynamics of the Two-Dimensional Spin-1/2 XY Model

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The generalized Trotter formula is used to map the two-dimensional spin-1/2 XY model onto several three-dimensional Ising models with complicated many-spin interactions. This hierarchy of Ising-like models is studied by means of analytic and Monte Carlo techniques. We demonstrate that the sequence of these Ising models can be used to calculate accurately the thermodynamics of the two-dimensional spin-1/2 XY model. By calculating the specific heat, spin correlation functions, susceptibilities and a disorder parameter, we address the question of the nature of the phase transition in the two-dimensional spin-1/2 XY model.

I. Introduction

Although it is well-known that there cannot exist long-range order in the two-dimensional spin-1/2 XY model at non-zero temperature [1], high-temperature series expansions [2, 3] suggest the existence of critical behavior. For classical versions of the model (planar rotator models) it is well-established that although there is no spontaneous magnetization there is a phase transition at non-zero temperature [4, 5]. This phase transition is attributed to the existence of topological excitations in the system and has been studied extensively [6–13]. The physical picture is that apart from the usual spin waves also topological defects (spin vortices) are important. At sufficiently low temperature vortex anti-vortex pairs are bound and it is the unbinding of pairs of these defects with increasing temperature that causes a phase transition to take place.

Whether or not the same physical picture can be extended to the two-dimensional spin-1/2 XY model is an open question. It is known that in two dimensions nonuniversal behavior is not unusual [14]. In particular it has been suggested that for this type of models the universality class depends on the spin [2, 3]. Therefore results for the *classical* 2D *planar* model should not be taken as a criterion for the calculations of the two-dimensional spin-1/2 XY model [2]. In comparison with the classical model, much less is known about the quantum model mainly because most techniques which have been successfully applied to the classical model become much less reliable when extended to the spin-1/2 case [15–21].

We will calculate the thermodynamic properties of the two-dimensional spin-1/2 XY model by exploiting the formal analogy between d-dimensional quantum spin systems and $(d+1)$-dimensional Ising-spin models [22]. Using the generalized Trotter formula, Suzuki showed that $Z=\mathrm{Tr}\,\exp(-\beta H)=\lim_{m\to\infty} Z_m$ where

$$Z_m \equiv \mathrm{Tr}\left[\prod_{\langle ij\rangle} \exp\left(-\frac{\beta}{m} H_{i,j}\right)\right]^m, \tag{1.1}$$

will be called the m-th approximation to the partition function Z, $H_{i,j}$ is any two-site spin-1/2 Hamiltonian chosen such that $H=\sum_{\langle ij\rangle} H_{i,j}$ and the product in (1.1) runs over some ordered set of nearest-neighbor bonds of the lattice [22]. For the two-dimensional spin-1/2 XY model on a square lattice we have

$$H_{i,j} = -J(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y), \tag{1.2}$$

where σ_i is the Pauli spin-operator at site $i(\sigma_j^\alpha \sigma_k^\beta = i\delta_{j,k}\varepsilon_{\alpha\beta\gamma}\sigma_j^\gamma)$ and the exchange interaction J can always be taken to be one [2]. For convenience we

will assume periodic boundary conditions in all our calculations. Our goal is to calculate the thermodynamic properties of the approximation (1.1) and to study the convergence of the results as a function of m. It is important to note that in general the results for Z_m and the related approximants for the thermodynamic quantities depend on the particular order chosen for the product of operators in (1.1). Although in the limit $m\to\infty$ results are independent of m, a careful examination of the different possibilities is desirable, as it turns out that some orderings are easier to handle than other ones, and because the rate of convergence may depend on the choice of ordering.

We will carry out this program in two steps. First we will discuss the properties of a class of $m=1$ approximations. This type of approximation for the partition function of spin-1/2 Heisenberg model was introduced by Suzuki who called it the pair-product model [23]. As pointed out by Suzuki the mathematical properties of the pair-product model are very similar to that of the original quantum model. Suzuki analysed the pair-product model for the Heisenberg model by using the Bethe approximation and Padé approximation techniques [23]. Hubbard has reviewed the application of similar approximations to the 3D Hubbard model [24]. We will discuss a large class of pair-product approximations for the two-dimensional spin-1/2 XY model that can be solved rigorously and we will refer to this approximation as the independent pair approximation (IPA) [25]. The IPA yields results which are not in conflict with known rigorous results. This is due to the fact that even in the IPA no essential model property (such as rotational spin-symmetry) of the two-dimensional spin-1/2 XY model is lost.

Secondly we will go beyond the $m=1$ approximation by choosing a quite different scheme of ordering of the two-site Hamiltonians $H_{i,j}$ than the one that was used to solve the $m=1$ approximation analytically. In going beyond the $m=1$ approximation we have not found it possible to analyse the approximations analytically and we have to resort to Monte Carlo simulation techniques [26] in order to obtain numerical results. Brief reports on parts of the work presented in this paper can be found in [27].

II. Independent Pair Approximation

In order to prove that it is possible to solve particular $m=1$ approximations rigorously we make a graphical construction [25] that maps these representations onto a rigorously solvable two-dimensional lattice model, a staggered 8-vertex model (SEV). The resulting SEV satisfies the free-fermion condition and consequently it belongs to the class of staggered 8-vertex models that have been solved analytically [28]. The construction parallels the one used to map the checkerboard representation of one-dimensional spin-1/2 models onto an 8-vertex model [29]. The IPA to the partition function reads

$$Z_1 \equiv \mathrm{Tr} \prod_{\langle ij\rangle} \exp(-\beta H_{i,j}), \tag{2.1}$$

To proceed further it is necessary to choose a representation for the states in which we will evaluate the trace. In this section we will work with states of products of single spin states, whereby each single spin states is chosen to be an eigenstate of the z-component of the spin operator. Obviously there are two such eigenstates per site and we can label the eigenstates by means of Ising spin variables. We use the notation $\sigma_i^z|S_i\rangle = S_i|S_i\rangle$. As each spin of the square lattice interacts with four neighbors it is clear that by inserting resolutions of the identity we will end up with $4L^2$ Ising spins (L is the linear size of the square).

As shown in Fig. 1 we may place the four Ising spin variables on the corners of a small square that contains the corresponding quantum spin. Now we have to find a way to order the two-site operators such that all bonds are taken into account exactly once. Let us start by considering the two-site operator acting on the spins on site 1 and 2 (see Fig. 1). If we label the Ising spin variable by the number of the site enclosed by the elementary square and one of the letters a,b,c,d the matrix element for the bond 1–2 can be denoted by $\langle S_{1,a} S_{2,a'}| \exp(-\beta H_{1,2})|S_{1,b} \cdot S_{2,b'}\rangle$. As we are inserting resolutions of the identity it is obvious that the next time we encounter an interaction in which for instance the spin at site 2 participates, we have to use either $S_{2,a'}$ or $S_{2,b'}$ in the bra respectively ket of the corresponding matrix element. For example, if we take the interaction 2–3 into account it yields the matrix element

$$\langle S_{2,b'} S_{3,a''}| \exp(-\beta H_{2,3})|S_{2,c'} S_{3,b''}\rangle.$$

The notation used so far becomes very clumsy after taking a few bonds into account but one does not need to keep track of all the indices. To this end we introduce the convention that if we add a matrix element to the product under construction, we draw two arrows, pointing to the Ising spins that appear in the ket of the matrix element, on the edges of the squares that cross the bond (dashed lines in Fig. 1). Now the rule of successively using the Ising spins of a particular square is replaced by the requirement that the orientation in which the arrows run over

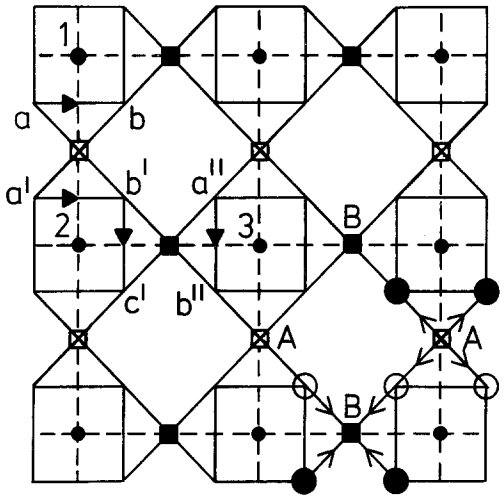

Fig. 1. The effective Ising lattice model for the $m=1$ approximation to partition function of the 2D spin-1/2 XY model. The original lattice is given by the dashed lines. The Ising spins live on the corners of the squares that surround the original lattice points. The equivalent staggered 8-vertex lattice consist of sublattices A and B

the squares cannot be changed. Note that once one of the Ising spins of a square is used in a bra or ket the orientation on the square is fixed. Using this notation we can walk over the lattice and add more and more exponents of two-site Hamiltonians to the list such that at the end there are exactly four arrows on each square (in the case of periodic boundary conditions). Then all Ising spins have been used twice (once in a bra and once in a ket) and the path-sum representation has been found. It is not difficult to convince oneself that this construction can be made for many (but not all) different orderings under the condition that L is even.

As for the one-dimensional case [29] we turn the Ising model into a vertex model by drawing diagonals in the squares between (instead of on) the elementary squares on which the Ising spins live, using the same convention for putting arrows on the lines through the corners and attaching the appropriate weights to the vertex configurations. From Figs. 1, 2 and the matrix representation for the two-body operator $\exp(-\beta H_{i,j})$

$$\langle S_i, S_j|\exp(-\beta H_{i,j})|\bar{S}_i, \bar{S}_j\rangle = e^{-\beta J}\begin{pmatrix} e^{2\beta J} & 0 & 0 & 0 \\ 0 & \cosh 2\beta J & \sinh 2\beta J & 0 \\ 0 & \sinh 2\beta J & \cosh 2\beta J & 0 \\ 0 & 0 & 0 & e^{2\beta J} \end{pmatrix}; \quad \begin{matrix} |-1\,-1\rangle \\ |\ 1\,-1\rangle \\ |-1\ \ 1\rangle \\ |\ 1\ \ 1\rangle \end{matrix}, \tag{2.2}$$

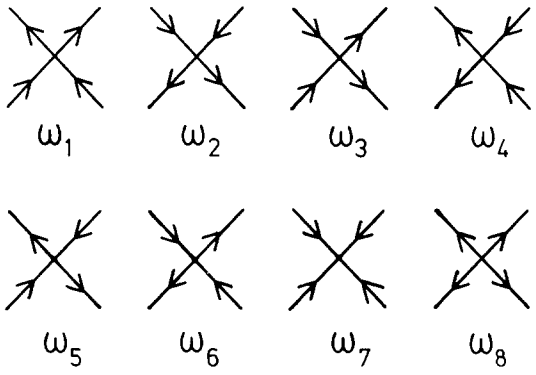

Fig. 2. The eight vertex configurations and their corresponding weights

it follows that the resulting vertex model is a SEV with weights given by

$$\omega_1=\omega_1'=\omega_2=\omega_2'=1, \tag{2.3a}$$

$$\omega_3=\omega_3'=\omega_4=\omega_4'=\sinh 2\beta J, \tag{2.3b}$$

$$\omega_5=\omega_7'=\omega_6=\omega_8'=\cosh 2\beta J, \tag{2.3c}$$

$$\omega_7=\omega_5'=\omega_8=\omega_6'=0, \tag{2.3d}$$

where $\omega_i(\omega_i')$ are the weights on the sublattice $A(B)$. The general solution for the staggered 8-vertex model is not known but a rigorous closed form expression for the free energy can be derived if the vertex weights obey the free-fermion condition [28]. For the two-dimensional spin-1/2 XY model this happens to be the case and the SEV approximation to the free energy per site of the two-dimensional spin-1/2 XY model reads

$$F_1^{\mathrm{SEV}}/L^2=-\frac{1}{8\pi^2\beta}\int_0^{2\pi}\int_0^{2\pi} d\phi\, d\theta \cdot \ln[4(1+y^2)^2-4y^2(\cos\theta+\cos\phi)^2], \tag{2.4}$$

where $y=\sinh 2\beta J$. From (2.4) we already see that the critical point must be at $y=1$ ($T_c/J\approx 2.27$) since then the integrand diverges for $\theta=\phi=0$. A more detailed analysis reveals that the specific heat has a logarithmic divergence at the Ising model critical temperature $\sinh(2J/T_c)=1$. It can be shown that the free-fermion condition remains satisfied if we add a field $\mathbf{h}=h\mathbf{e}_z$ and as can be expected on physical grounds, it follows that there is no spontaneous out-of-plane magnetization ($M^z=0$) nor a divergence in the out-of-plane susceptibility [25]. Thus the rigorous solution of the simplest approximation to the partition function of the two-dimensional spin-1/2 XY model yields results which are not in conflict with all known rigorous results on the model. The fact that the specific heat of the SEV approximation

to the two-dimensional spin-1/2 XY model is logarithmically divergent is in qualitative agreement with experimental results on $CoCl_2 \cdot 6H_2O$, an example of a 2D spin-1/2 XY magnet [30]. Recently a similar anomaly in the specific heat has also been observed in $BaCo_2(AsO_4)_2$, a prototype of a two-dimensional spin-1/2 XY model on a honeycomb lattice [31].

III. Monte Carlo Simulation

A. Theory

On the basis of the IPA it is impossible to answer the question whether the obtained critical behavior is not an artifact of the $m=1$ approximation, or whether it is due to choosing a particular ordering of the exponential operators in (1.1). We now examine the problem of extending the calculation to $m \geqq 1$ and other orderings. Extending the staggered 8-vertex formulation to $m>1$ is possible but it is certainly not the most promising approach if we have to use the Monte Carlo simulation method. As two out of eight vertex configurations are forbidden (see (2.3d)) it is not possible to employ a simple Monte Carlo scheme for changing the vertex configurations in an unbiased way. In this respect we would face at least the same difficulties as those encountered in simulations of one-dimensional quantum spin models [32–34]. We will not go into details about this because an extensive discussion of the fundamental and technical problems that arise in simulations of 1D spin-1/2 models (XY and Heisenberg models) can be found in [33] but only emphasize the fact that the higher the model symmetry, the harder it is to construct a correct and efficient simulation algorithm. In addition to this we would have to find an efficient scheme to deal with the complicated three-dimensional lattice structure. In view of all this we consider extensions of staggered 8-vertex formulations for $m>1$ as being impractical.

It is not hard to trace back the reason for the problems that appear in the 8-vertex type formulation. By working with a representation in which σ_i^z is diagonal, conservation of magnetization per two-site block requires that most of the elements of the two-site interaction matrix (2.2) are zero. Consequently it is difficult to find simple spin-flip algorithms satisfying these constraints and being able of generating *all* allowed configurations. In the case of the XY model (in zero external field $\mathbf{h}=0$) there is a representation of the spin-states such that eight out of the sixteen elements are strictly positive. Applying two successive cyclic permutations of the spin-components we find that the XY model turns into a XZ model

$$H = -J \sum_{\langle ij \rangle} (\sigma_i^x \sigma_j^x + \sigma_i^z \sigma_j^z). \tag{3.1}$$

Since a cyclic permutation is a unitary transformation the partition function does not change. It is straightforward to show that for the XZ model the two-site interaction matrix is given by

$$T(S_i, S_j; \bar{S}_i, \bar{S}_j) = \langle S_i S_j | \exp\left[\frac{\beta J}{m}(\sigma_i^x \sigma_j^x + \sigma_i^z \sigma_j^z)\right] | \bar{S}_i \bar{S}_j \rangle$$

$$= \delta_{S_i S_j, \bar{S}_i \bar{S}_j} (\tfrac{1}{2} \sinh 2K_m)^{1/2} \exp\left(K_m S_i \bar{S}_j + \frac{\beta J}{m} S_i S_j\right), \tag{3.2}$$

where $K_m = \frac{1}{2} \ln \coth(\beta J/m)$. From (3.2) it is clear that by making a rotation in spin space we have found a representation that does not suffer from the drawbacks of the representation used in previous simulations of 1D spin-1/2 system [32–34].

The remaining problem is to split up the Hamiltonian such that the labor involved in keeping track of all two-site interactions is not too exhaustive. We decompose the Hamiltonian as $H = H_h + H_v$ where $H_{h(v)}$ is a sum of non-interacting horizontal (vertical XZ chains. Then we can either choose the checkerboard or real-space partitioning to break-up the XZ chains into two-site blocks [22, 29, 32, 35]. In this last step we do the same as for the one-dimensional models, i.e. we sum out intermediate states [35] and instead of $4mL^2$ Ising-spin variables (4 per quantum spin because each quantum spin interacts with four other quantum spins) we have reduced the total number of variables by a factor of two. It is clear that this analytic reduction of the number of degrees of freedom is an essential step in the development of an efficient algorithm.

Following the prescriptions outlined above it is nothing but a tedious exercise in manipulating indices to rewrite the m-th approximant to the partition function of the two-dimensional spin-1/2 XY model as a three-dimensional Ising model with complicated many-spin interactions. We find [27]

$$Z_m = c(\sinh 2K_m)^{mL^2} \sum_{\{S_{i,j}^{(k)}\}}{}' \sum_{\{\bar{S}_{i,j}^{(k)}\}}{}' \prod_{k=1}^{m} \prod_{j=1}^{L} \prod_{i=1}^{L} h(j,k)\, v(i,k), \tag{3.3}$$

where c is a numerical constant. The prime on the summation symbols means that the sums over the Ising spin variables are restricted by $2mL-1$ constraints that can be written as

$$\bar{S}_{1,1}^{(k)} = S_{1,1}^{(k)} \prod_{i=2}^{L} S_{i,1}^{(k)} S_{i,1}^{(k+1)} \prod_{i=2}^{L} \prod_{j=2}^{L} \bar{S}_{i,j}^{(k)} S_{i,j}^{(k+1)}, \tag{3.4a}$$

$$\bar{S}^{(k)}_{1,j}=S^{(k)}_{1,j}\prod_{i=1}^{L} S^{(k)}_{i,j}\bar{S}^{(k)}_{i,j}; \quad j>1, \tag{3.4b}$$

$$\bar{S}^{(k)}_{i,1}=S^{(k)}_{i,1}\prod_{j=1}^{L} \bar{S}^{(k)}_{i,j}S^{(k+1)}_{i,j}; \quad i>1, \tag{3.4c}$$

$$S^{(k)}_{1,1}=S^{(1)}_{1,1}\prod_{i=2}^{L}\prod_{j=1}^{L} S^{(1)}_{i,j}S^{(k)}_{i,j}\prod_{j=2}^{L} S^{(1)}_{1,j}S^{(k)}_{1,j}; \quad k>1. \tag{3.4d}$$

For periodic boundary conditions and real-space split-up of the XZ chains $h(j,k)$ is given by

$$h(j,k)=\cosh\Big[K_m(S^{(k)}_{1,j}\bar{S}^{(k)}_{1,j}+\ldots+S^{(k)}_{1,j}\ldots S^{(k)}_{L,j}\bar{S}^{(k)}_{1,j}\ldots\bar{S}^{(k)}_{L,j}) +\frac{\beta J}{m}(S^{(k)}_{1,j}S^{(k)}_{2,j}S^{(k)}_{3,j}\bar{S}^{(k)}_{1,j}+\ldots+S^{(k)}_{1,j}\ldots S^{(k)}_{L,j}\bar{S}^{(k)}_{1,j}\ldots\bar{S}^{(k)}_{L-2,j})\Big] \times\exp\Big[\frac{\beta J}{m}(S^{(k)}_{1,j}S^{(k)}_{2,j}+S^{(k)}_{1,j}\ldots S^{(k)}_{L,j}\bar{S}^{(k)}_{2,j}\ldots\bar{S}^{(k)}_{L-1,j})\Big], \tag{3.5}$$

whereas for periodic boundary conditions and checkerboard break-up

$$h(j,k)=\cosh[K_m(S^{(k)}_{1,j}\bar{S}^{(k)}_{1,j}+\ldots+S^{(k)}_{1,j}\ldots S^{(k)}_{L,j}\bar{S}^{(k)}_{1,j}\ldots\bar{S}^{(k)}_{L,j})] \cdot\exp\Big[\frac{\beta J}{m}(S^{(k)}_{1,j}S^{(k)}_{2,j}+S^{(k)}_{3,j}S^{(k)}_{4,j}+\ldots+S^{(k)}_{L-1,j}S^{(k)}_{L,j}\Big] \cdot\exp\Big[\frac{\beta J}{m}(\bar{S}^{(k)}_{2,j}\bar{S}^{(k)}_{3,j}+\bar{S}^{(k)}_{4,j}\bar{S}^{(k)}_{5,j}+\ldots+\bar{S}^{(k)}_{L,j}\bar{S}^{(k)}_{1,j}\Big]. \tag{3.6}$$

The corresponding expressions for $v(i,k)$ are obtained from $h(j,k)$ by replacing the symbols $S^{(k)}_{l,j}\to\bar{S}^{(k)}_{i,l}$ and $\bar{S}^{(k)}_{l,j}\to S^{(k+1)}_{i,l}$. The 3D model (3.3) has complicated many-spin interactions and a coupling that depends on the lattice size in the Trotter direction (labeled by the superscript k). Note that starting from (3.4) we label the spins by x- and y-coordinates (i,j) whereas in the equations preceeding (3.4) we used only one index per lattice site in order to keep the notation simple.

During a simulation we want to sample the energy ($E=\lim_{m\to\infty} E_m$, $E_m=-\partial\ln Z_m/\partial\beta$), specific heat ($C=\lim_{m\to\infty} C_m$, $C_m=-\beta^2\partial E_m/\partial\beta$) and spin correlation functions that change drastically if the system undergoes a phase transition (assuming that there is one). It has been noted previously that in models that exhibit a phase transition without long-range order (such as the 2D XY model) it is more convenient to study *disorder* parameters than to look for quantities that describe the degree of order [14]. Moreover in models which are self-dual (such as the 2D Ising model) disorder and order are intimately related to each other. A correlation function that we have measured in our simulations is

$$D=L^{-2}\sum_{i,j=1}^{L}\langle D_a(i,j)\,D_b(i,j)\rangle, \tag{3.7a}$$

where

$$D_a(i,j)=(1-\sigma^x_{i,j}\sigma^x_{i+1,j+1}-\sigma^z_{i,j}\sigma^z_{i+1,j+1}), \tag{3.7b}$$

and

$$D_b(i,j)=(1-\sigma^x_{i,j+1}\sigma^x_{i+1,j}-\sigma^z_{i,j+1}\sigma^z_{i+1,j}). \tag{3.7c}$$

In studies of the classical analogon, the planar rotator model, correlation function (3.7) gives information about the occurrence of vortex-like excitations [36]. Therefore we will call D a vortex detector although we do not know of any simple intuitive picture for vortex-like excitations in the quantum system.

A definite advantage of working with the representation (3.3) is that we can measure the thermal energy, specific heat and any spin-spin correlation function simultaneously. As we have taken the eigenstates of $\sigma^z_{i,j}$ as the representation for the states of the system it is obvious that it is easy to calculate correlation functions of the $\langle\sigma^z_{i,j}\sigma^z_{i',j'}\rangle$ type ($S^{(k)}_{i,j}S^{(k)}_{i',j'}$ correlation functions of 3D Ising model (3.3)). If we want to know $\langle\sigma^x_{i,j}\sigma^x_{i',j'}\rangle$ things are much more complicated because $\sigma^x_{i,j}$ changes the total magnetization of a state. Assume that the system is in a allowed state (i.e. the state has a weight which is strictly greater than zero). If we would have chosen to work with representations for which the matrix form of the two-body operator is of the type (2.2), applying the operator $\sigma^x_{i,j}\sigma^x_{i',j'}$ always yields a forbidden state (i.e. a state with zero weight in the partition function) if $i\neq i'$ or $j\neq j'$. If however we are using representation (3.1-6) things are quite different. From (3.2) it follows immediately that we can flip either the two Ising spins of the bra or the two Ising spins of the ket. Combined with the cyclic permumation property of the trace this leads to the condition that the number of spin flips within a row (column) must be even. Using the properties of the spin-1/2 operator algebra we can write

$$\langle\sigma^x_{i,j}\sigma^x_{i',j'}\rangle=\langle\sigma^x_{i,j}\sigma^x_{i,j'}\sigma^x_{i,j'}\sigma^x_{i',j'}\rangle, \tag{3.8}$$

but in general any string of σ^x operators that takes us from site (i,j) to site (i',j') would do as long as the "path" that brings us from site (i,j) to site (i',j') is made up of horizontal and vertical bonds. In practice we use expressions

$$\langle\sigma^x_{i,j}\sigma^x_{i',j'}\rangle=Z^{-1}\,\mathrm{Tr}\,\sigma^x_{i,j}\sigma^x_{i,j'}e^{-\beta H}\sigma^x_{i,j'}\sigma^x_{i',j'}, \tag{3.9a}$$

$$\langle\sigma^y_{i,j}\sigma^y_{i',j'}\rangle=Z^{-1}\,\mathrm{Tr}\,\sigma^z_{i,j}\sigma^x_{i,j}\sigma^x_{i,j'}e^{-\beta H}\sigma^x_{i,j'}\sigma^x_{i',j'}\sigma^z_{i',j'}, \tag{3.9b}$$

to "measure" all x−x and y−y correlation functions. From the correlation functions we also calcu-

late the $(\mathbf{q}-(0,0))$ in-plane structure factor

$$S_{\|}=L^{-2}\sum_{i,j,i',j'=1}^{L}(\langle\sigma^x_{i,j}\sigma^x_{i',j'}\rangle+\langle\sigma^z_{i,j}\sigma^z_{i',j'}\rangle), \tag{3.10a}$$

and the $(\mathbf{q}-(0,0))$ out-of-plane structure factor

$$S_{\perp}=L^{-2}\sum_{i,j,i',j'=1}^{L}\langle\sigma^y_{i,j}\sigma^y_{i',j'}\rangle. \tag{3.10b}$$

These structure factors can give us direct information about the existence of long-range correlations in the system.

For quantum systems the static response of a physical quantity described by the operator B on a small external perturbation described by an operator A is given by the static (Kubo) susceptibility

$$\chi_{A,B}\equiv\int_0^{\beta}d\lambda\langle e^{\lambda H}A^{\dagger}e^{-\lambda H}B\rangle-\beta\langle A^{\dagger}\rangle\langle B\rangle. \tag{3.11}$$

As we are dealing with a quantum system, the relation $\chi_{A,B}=\beta(\langle A^{\dagger}B\rangle-\langle A^{\dagger}\rangle\langle B\rangle)$ which is valid for a classical system does not hold anymore unless $A(B)$ is a conserved quantity (then $A(B)$ commutes with H). In our case $\sum_{i,j=1}^{L}\sigma^y_{i,j}$ is a conserved quantity and therefore we know $\chi_{\perp}$ because we can calculate $S_{\perp}$. We have not yet found a practical method to calculate directly the in-plane static susceptibility $\chi_{\|}$ of model (3.1). However there is a way to calculate bounds on $\chi_{\|}$. By making use of rigorous inequalities [37, 38] we can show that

$$f(y)\leqq\chi_{\|}/\beta S_{\|}\leqq 1, \tag{3.12a}$$

where the function $f(y)$ is defined implicitly by

$$y=x\tanh x=\beta J S_{\|}^{-1}(\langle\sigma^x_{0,0}\sigma^x_{0,1}\rangle-\langle\sigma^y_{0,0}\sigma^y_{0,1}\rangle), \tag{3.12b}$$

and

$$f(y)=x^{-1}\tanh x. \tag{3.12c}$$

There are two limits for which (3.12) turns into the equality $\chi_{\|}=\beta S_{\|}$. The first (trivial) case is the high temperature limit $\beta\to 0$. Second, if there is a critical temperature for which $S_{\|}\to\infty$, then $x\to 0$ and consequently $f(y)\to 1$. It is well established that for the planar rotator model, which is the classical analogon of the two-dimensional spin-1/2 XY model, $S_{\|}$ is divergent at and below the Kosterlitz-Thouless transition temperature. Thus if the quantum $S_{\|}$ behaves qualitatively the the same as its classical counterpart, then below T_c we have $\chi_{\|}=S_{\|}=\infty$. Moreover above T_c, β is relatively large, and consequently f will deviate little from 1.

The above discussion applies to the infinite system. As we can only simulate finite systems we must verify explicitly how good the bounds on $\chi_{\|}$ are. For the two-dimensional spin-1/2 XY model, we can calculate all quantities that enter the right-hand side inequality of (3.12b) by means of the Monte Carlo technique and in this way we will get estimates for the bounds on $\chi_{\|}$.

B. Simulation Technique

At this point we have reformulated the problem of calculating the m-th approximant to the partition function such that we are in the position to apply the standard Metropolis Monte Carlo method [26]. It is well-known that this Monte Carlo technique cannot be used to calculate the (approximant to the) partition function itself [26] but it can be used to calculate estimators for the expectation values of observables. In practice we have to implement the Metropolis algorithm for the unnormalized probability function

$$f(\{S^{(k)}_{i,j}\},\{\bar{S}^{(k)}_{i,j}\})=\prod_{k=1}^{m}\prod_{j=1}^{L}\prod_{i=1}^{L}h(j,k)\,v(i,k). \tag{3.13}$$

subject to the constraints (3.4). Note that due to the constraints (3.4a–d) there are (Ising) spin configurations that are forbidden and for which the above function must be set to zero. However, there are no spin configurations for which $f<0$, which relieves us from a fundamental problem usually encountered when applying Monte Carlo techniques to fermion systems. It is easy to see that we can flip any single Ising spin that does not appear in the left-hand side of (3.4) and (3.4) will tell us which other spins we have to change. Although several spins change at the same time (Monte Carlo step) we still call this a single-spin flip procedure. Since we change several spins at each step one might think that because of the highly non-local interactions in (3.13) or (3.14), one Monte Carlo step will take much computing time. This would certainly be the case if we would use one computer storage unit (i.e. a word) per spin variable because we would have to make several loops to update spins and calculate the transition probability. As we are simulating an Ising model we may as well use one bit to store an Ising spin and pack each row and column into one word. Then updating many spins in one row or column means that we can use masking operations (AND, OR and EXLUSIVE OR) on words. Boolean operations on integer variables are not supported by standard Fortran 77 compilers but most Fortran compilers (on

DEC, CDC and IBM machines) allow for this kind of operations and produce extremely efficient code. The use of this technique is necessary to get acceptable program performance but it is clear that simulation of the 2D XY model will take much more time than simulating a normal 3D Ising model (with nearest-neighbor interactions) of the same size.

We have tested the single-spin flip algorithm by simulating small systems (up to 3×3) and have compared the data with results obtained from exact enumerations and diagonalizations and found excellent agreement. In going to larger lattices (6×6) we observed that for high temperatures, the data deviated systematically from the high-temperature series results [3, 16]. The Monte Carlo algorithm itself also signalled that something was going wrong because the acceptance rate became extremely small. From (3.14) or (3.15) it follows that if K_m is large, and this happens if $T \to \infty$ or $m \to \infty$, changing spins without keeping the prefactor of K_m constant is very difficult. A simple way out of this problem is to flip the set of spins

$$\{S_{i,j}^{(1)}, \ldots, S_{i,j}^{(m)}, \bar{S}_{i,j}^{(1)}, \ldots, \bar{S}_{i,j}^{(m)}\}.$$

Such a multi-spin flip step keeps (3.4) intact and also requires less computing time.

Combination of the single-spin flip procedure with the multi-spin flip procedure yields a Monte Carlo scheme that reproduces all known (i.e. small systems, high-T) results of the two-dimensional spin-1/2 XY model. In practice we found that the "classical" multi-spin flip step was the most important in the sense that it was sufficient to keep the ratio, single-spin flips over multi-spin flips, low (10%). All data presented in this paper have been obtained from at least two independent runs of 10000 Monte Carlo steps per Ising spin each. The CPU-time required for such runs depends on the size of the system and on the number of quantities that we want to "measure". Especially the calculation of spin-correlation functions is a very time-consuming procedure because it requires of the order of L^4 operations (Monte Carlo itself requires of the order of L^2 operations). Simulation of a $L=16$, $m=8$ ($16 \times 16 \times 8$, 4096 Ising spins) system without calculating all spin correlations takes 90 min of CPU-time on a CDC 170/750. For the largest systems ($L=24, 32$, $m=4$) for which we have calculated all spin correlation functions it was necessary to use a CYBER 205. Efficient use of the vector processor for this type of problem was possible because the most CPU-intensive code, the calculation of the spin correlations, could be vectorized to a very high degree (for $L=32$ we gained a factor of about 65 compared to the program running in scalar mode). In this way the CPU time was effectively reduced to that of the Monte Carlo algorithm. A typical $L=24$, (32), $m=4$ simulation takes approximately 50(100) min on a (one-pipeline) CYBER 205 machine.

IV. Simulation Results

Guided by the rigorous $m=1$ result (for a different ordering) that there is a phase transition at $T_c/J \approx 2.27$, we first perform simulations of systems of different size for $m=1$. In Fig. 3 we show $m=1$ results for the energy per site, obtained from the IPA, checkerboard and real-space representation. We see that the results for the three different orderings are almost the same unless the temperature $T/J < 2.25$. Also the size dependence (for $L \geqq 6$) is rather weak. At low temperature $T/J=1$ the approximate energy E_1 is much lower than the rigorous lower bound $E_0/JL^2 \geqq -2.25$ [39] but since the XZ real-space approach yields energies which are systematically higher than those of the checkerboard approximation we decided to use the real-space approximation in most of our simulation. As in the 1D case, for the two-dimensional spin-1/2 XY model the real-space approximation is more accurate than the checkerboard approximation [35]. In Fig. 4 we depict simulation data for the $m=1$ approximant (C_1) to the specific heat. At $K \approx K_1^c$ the specific heat exhibits a maximum that grows slowly with the lattice size. This is not inconsistent with the exact $m=1$ solution

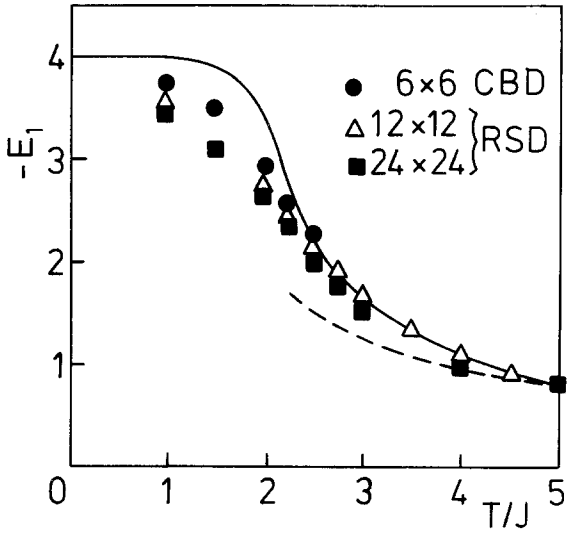

Fig. 3. Energy per site of the 2D spin-1/2 XY model in the $m=1$ approximation. Solid line: rigorous staggered 8-vertex solution, full circles: checkerboard decomposition (CBD), full squares and open triangles: real-space decomposition (RSD) and broken line: high-temperature expansion

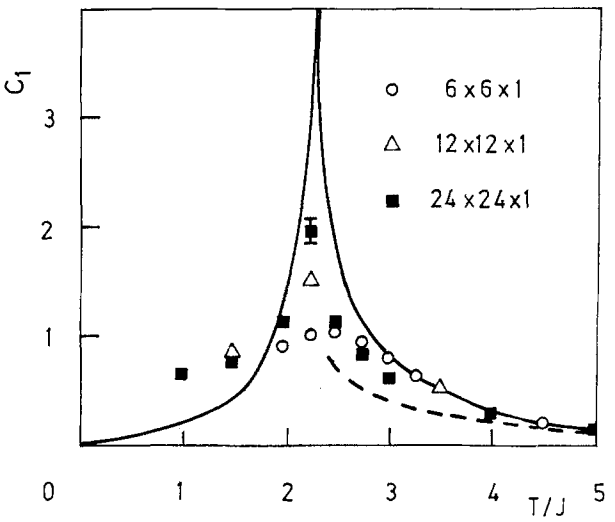

Fig. 4. Specific heat per site of the 2D spin-1/2 XY model in the $m=1$ approximation. Solid line: rigorous staggered 8-vertex solution, open circles, full squares and open triangles: real-space decomposition (RSD)

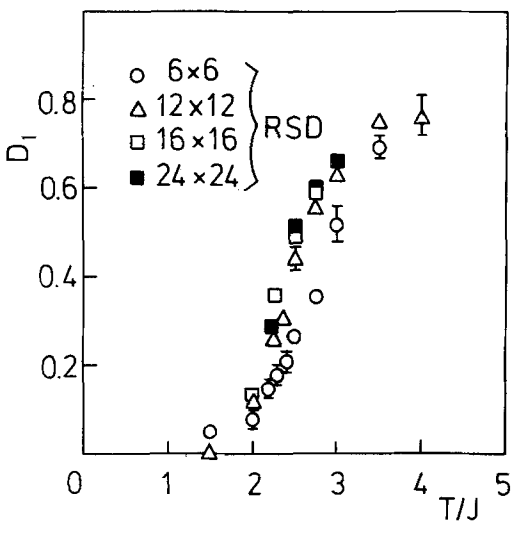

Fig. 5. The vortex correlation function in the $m=1$ real-space approximation

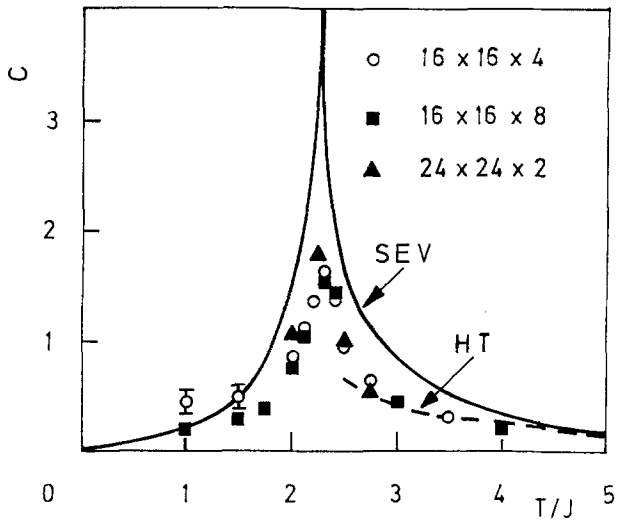

Fig. 6. Specific heat per site of the 2D spin-1/2 XY model. Solid line: rigorous staggered 8-vertex solution; broken line: high-temperature expansion. Comparison with the data of Fig. 1 shows that in the critical region the m-dependence is very weak

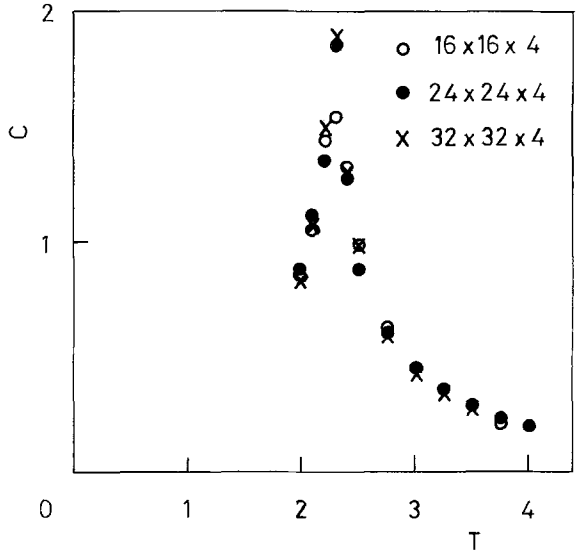

Fig. 7. Specific heat per site of the 2D spin-1/2 XY model obtained from simulations of systems of different size and $m=4$. The $16\times16\times4$ data is not the same as the $16\times16\times4$ data shown in Fig. 6

for the SEV which predicts a logarithmically divergent specific heat [25]. From our $m=1$ simulation data we may infer that the phase transition in the IPA is not the result of choosing a particular ordering. The first simulation of the two-dimensional spin-1/2 XY model was reported by Suzuki et al. who only studied the $m=1$ case [32]. Their simulation data for the specific heat disagree with ours and is also in qualitative disagreement with our rigorous $m=1$ solution. This is probabily due to the fact that the Monte Carlo scheme employed by Suzuki et al. cannot generate all states of the effective 3D Ising model [32].

The temperature dependence of the $m=1$ vortex-detector is shown in Fig. 5. It is clear that D_1 changes rapidly if T approaches T_c indicating that the system might exhibits a peculiar kind of disorder if $T \geqq T_c$. We find that for $L \geqq 8$ the size dependence of D_1 is small. By increasing m we can improve the approximation systematically. From the $m>1$ data shown in Figs. 6, 7 we conclude that for $T/J>2$ the specific heat, which from point of view of conver-

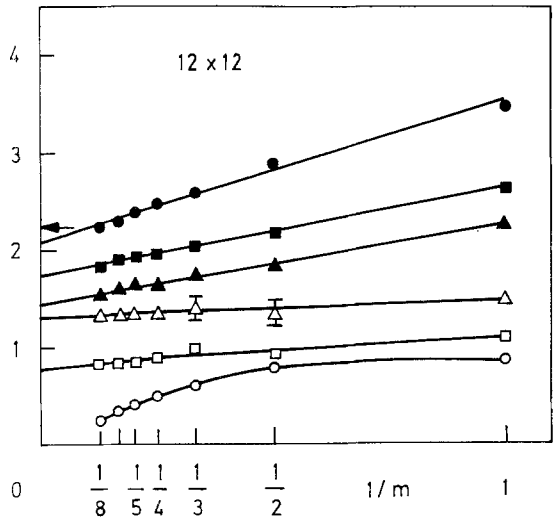

Fig. 8. Minus the energy per site (full symbols) and specific heat per site of the 2D spin-1/2 XY model (open symbols) as a function of $1/m$. Circles: $T/J=1$; squares: $T/J=2$ and triangles $T/J=2.25$. The arrow gives Pearsons estimate of the groundstate energy

gence is the most difficult quantity to calculate, depends weakly on the particular value of m. The $16\times16\times4$ data shown in Fig. 6 and $16\times16\times4$ data shown in Fig. 7 are not identical as they have been obtained from statistically independent runs of different programs (scalar and vectorized code) on different machines (VAX 11/780 versus CYBER 205).

For $T/J\geqq2$ and $L\geqq16$ the size dependence of specific heat per site is small. More convincing evidence that the convergence of the energy and specific heat is very good is given in Fig. 8. In the critical region ($T/J\approx2.27$) the m-dependence of physical quantities is very weak. Therefore it might be tempting to assume that to a good approximation the critical properties of the two-dimensional spin-1/2 XY model are that of the $m=1$ representation. Although our numerical data are not inconsistent with this assumption we take the point of view that the subtle β/m dependence of the approximants could change the critical behavior. Furthermore it is obvious that it is impossible to prove or disprove by means of Monte Carlo data whether or not a physical quantity is continuous or divergent. In particular it is impossible to decide from the simulation data that the specific heat diverges logarithmically.

Simulation data for the approximant D_m are shown in Fig. 9. Again we see the very rapid change in disorder if T approaches T_c. As for the energy and specific heat, in the critical region the m-dependence of D_m is very weak. Within the statistical accuracy of the simulation we find that $D_m\approx0$ if $T\to0$. This is in agreement with results of small-lattice calculations [40] although one should take into account that the

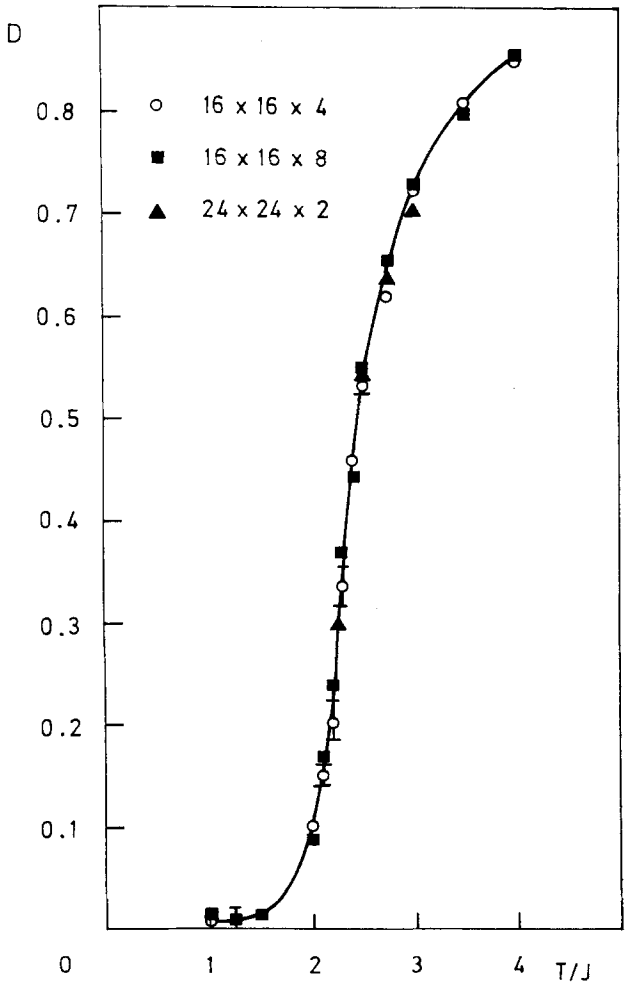

Fig. 9. The vortex correlation function, which measures the degree of disorder in the 2D spin-1/2 XY model, for lattices of different size and different m. In the critical region the m-dependence of this correlation function is very weak

vortex operators used in [40] differ from the one used in the present work. In Fig. 10 we plot the results for the in-plane structure factor $S_{\|}$. If there are no long-range correlations in the system we expect that this structure factor is independent of the number of sites (for a system of reasonable size). If there are long-range correlations (this does not imply long-range order), the structure factor should exhibit some functional dependence on the number of sites, i.e. it becomes extensive. From Fig. 10 we learn that the in-plane structure factor of the two-dimensional spin-1/2 XY model displays this behavior very clearly. According to (3.12) we can calculate bounds on the out-of-plane static susceptibility by evaluating the function $f(y)$. In Table 1 we collect some typical results. As anticipated previously, in the critical region $f(y)\approx1$ and therefore we may claim to have calculated $\chi_{\|}$ with the same accuracy as $S_{\|}$. The out-of-plane structure factor $S_{\perp}$

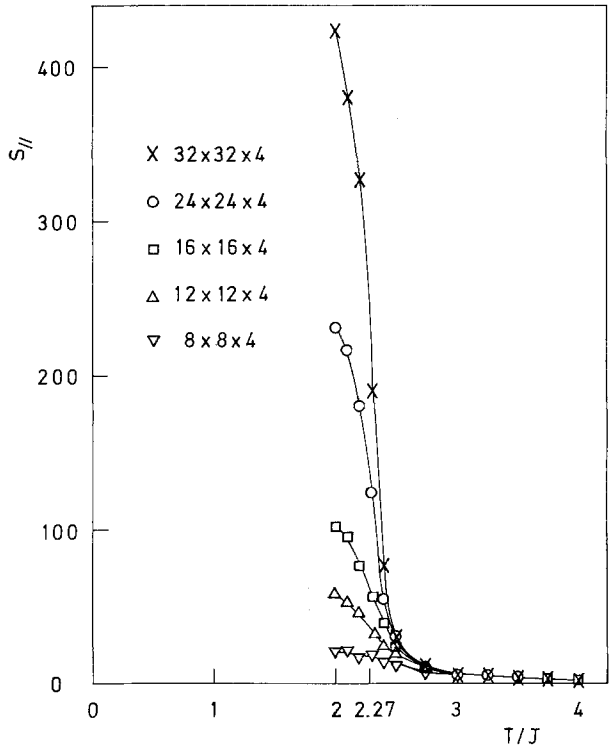

Fig. 10. The in-plane structure factor $S_{\|}$ of the 2D spin-1/2 XY model for lattices of different size as a function of the temperature. Solid lines are merely guides to the eye

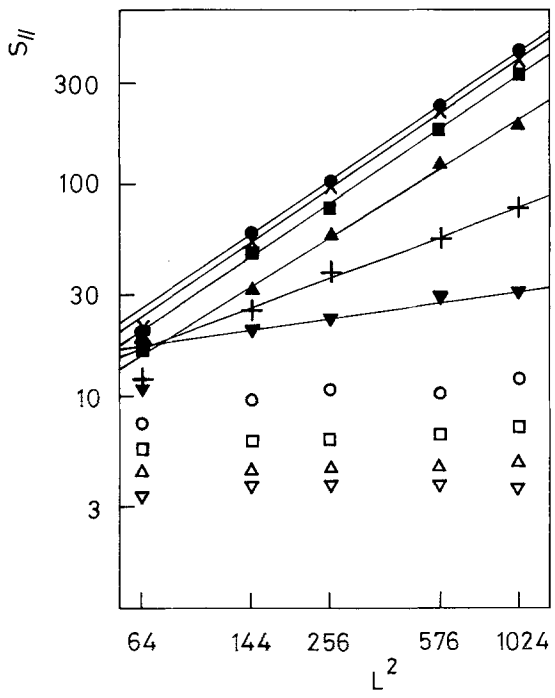

Fig. 11. Log-log plot of $S_{\|}$ as a function of L^2 indicating that for $T/J \leqq 2.5$, $S_{\|} \sim aL^{2b(T)}$ to a good approximation if we disregard the $L=8$ data (●: $T/J=2$, ×: $T/J=2.1$, ■: $T/J=2.2$, ▲: $T/J=2.3$, +: $T/J=2.4$, ▼: $T/J=2.5$, ○: $T/J=2.75$, □: $T/J=3$, △: $T/J=3.25$, ▽: $T/J=3.5$)

Table 1. Typical ($m=4$) results for the quantities entering (3.12) from which we obtain bounds on the out-of-plane susceptibility $\chi_{\|}: f(y) \leqq \chi_{\|}/\beta S_{\|} \leqq 1$

T	L	$S_{\|}$	$\langle\sigma^x_{0,0}\sigma^x_{0,1}\rangle$	$\langle\sigma^y_{0,0}\sigma^y_{0,1}\rangle$	$y=x\tanh x$	$f(y)$
2.00	12	59.8	0.49	−0.09	0.019	0.994
	16	101.7	0.48	−0.09	0.011	0.996
	24	226.6	0.48	−0.09	0.005	0.998
	32	424.3	0.49	−0.09	0.003	0.999
2.30	12	30.3	0.41	−0.08	0.028	0.991
	16	55.7	0.40	−0.07	0.015	0.995
	24	124.5	0.39	−0.06	0.006	0.998
	32	180.6	0.39	−0.06	0.004	0.999
2.75	12	9.4	0.28	−0.04	0.051	0.983
	16	10.7	0.28	−0.04	0.043	0.986
	24	10.2	0.28	−0.04	0.038	0.985
	32	12.1	0.28	−0.04	0.038	0.987

which is always an intensive quantity, is rather small (less than 1) and increases slowly with temperature (at least for $2 \leqq T/J \leqq 5$). This is consistent with the picture that in the two-dimensional spin-1/2 XY model, the spins are forced in the XY-plane (XZ-plane in the representation that we use for our simulations).

We will now examine the possibility of extracting additional information about the critical properties of the two-dimensional spin-1/2 XY model by making assumptions about the size dependence of $S_{\|}$. The strong size dependence of $S_{\|}$ for $T/J \leqq 2.4$ (see Fig. 10) indicates that $S_{\|} \sim aL^{2b(T)}$ [9]. In Fig. 11 we present a log-log plot of $S_{\|}$ as a function of L^2. This plot suggest that we should exclude our data for the smallest lattice ($L=8$) from this type of analysis. Least-square fits of the remaining data reveal that $S_{\|} \sim aL^{2b(T)}$ gives an excellent description of the data for $T/J \leqq 2.4$ (coefficient of determination >0.99). Analysis of high-temperature series for the two-dimensional spin-1/2 XY model favours a phase transition with conventional power law critical singularities [3]. We can test whether our data are compatible with this behavior by using finite-size scaling [41], i.e. we assume that

$$\chi_{\|} = L^{\gamma/\nu} G(L^{1/\nu}|T - T_c|\, T_c^{-1}), \tag{4.1}$$

where G is the so-called scaling function, γ is the susceptibility exponent and ν is the correlation-length exponent. According to the high-T series $T_c/J \approx 1.56$, $\gamma \approx 2.50$ and $\nu \approx 1.43$ [3]. Using these numbers (4.1) yields a function G which does not seem to have any scaling properties at all. Adjusting the critical temperature to the SEV result ($T_c/J \approx 2.27$) gives the results depicted in Fig. 12. In all our finite-size scaling plots based upon (4.1) we only used data for $T \geqq T_c$ as the data for $T < T_c$ did

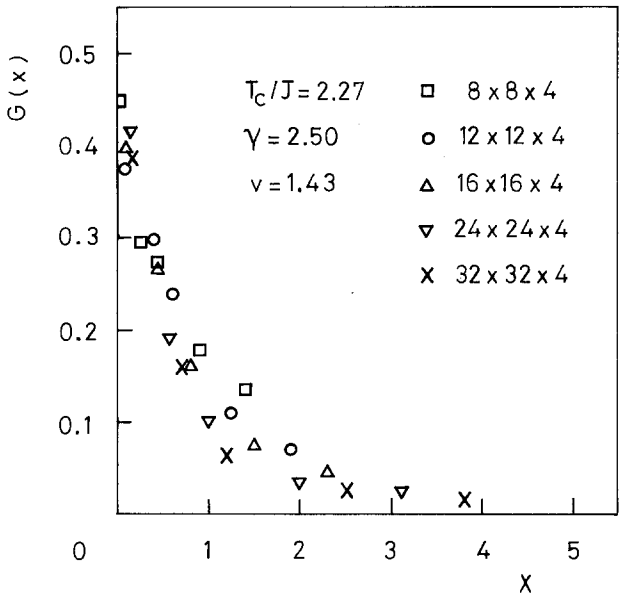

Fig. 12. The scaling function G (see (4.1)) obtained by assuming that the exponents γ and ν are given by the high-temperature series estimates of [3]

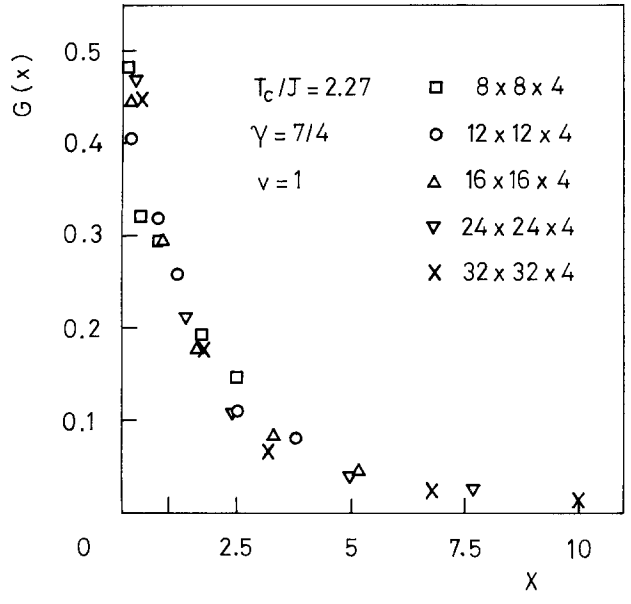

Fig. 13. The scaling function G (see (4.1)) obtained by assuming that the exponents γ and ν are that of the 2D Ising model

not show any sign of scaling behavior of the type (4.1). As G looks like a scaling function we might be tempted to say that our data are compatible with the critical exponents estimated from the high-T series. In Fig. 13 we show G obtained by assuming 2D Ising model exponents, i.e. $\gamma = 7/4$ and $\nu = 1$. Comparing Figs. 12 and 13 it seems as if the latter choice of exponents gives a "nicer" scaling function G than the former one. We have made a number of this type of scaling plots and we find that we can always find a nice looking scaling plot if we choose γ and ν such that $1.75 \leqq \gamma/\nu \leqq 2$ and $1 \leqq \nu \leqq 1.5$ (we have confined our search for scaling to the intervals $1.5 \leqq \gamma/\nu \leqq 3$, $0.5 \leqq \nu \leqq 3$). We have also calculated G by using critical exponents $\gamma = \infty$, $\nu = \infty$, $\gamma/\nu = 2 - \eta$, and $\eta = 1/4$ of the classical planar rotator model [7] and we find that G is not a scaling function. Although our data for $T \geqq T_c$ can be fitted with (4.1), this scaling ansatz cannot be used to extract from the Monte Carlo data reliable estimates for the critical exponents of the two-dimensional spin-1/2 XY model.

Analysis of Monte Carlo data of the classical planar rotator model reveals that, in contrast with usual second-order phase transitions, the specific heat has a maximum well above the temperature where the correlation length diverges [11, 12]. Our Monte Carlo results for the two-dimensional spin-1/2 XY model suggest that the estimate of the critical temperature based upon the position of the specific-heat peak agrees with the 2D Ising model value ($\sinh 2J/T_c = 1$) and also agrees with the critical temperature obtained from the behavior of the in-plane structure factor and the vortex detector.

By construction our technique cannot be used to calculate $T = 0$ properties because the Trotter-Suzuki formula requires that we have to take the limit $m \to \infty$ before we let $T \to 0$. Nevertheless we can carry out simulations in the low-temperature regime and try to extrapolate the results to $T = 0$. In Table 2 we give some results for the thermal energy of 8×8 systems for temperatures down to $T/J = 0.5$. The value of m has been taken such that the systematic error due to the Trotter formula is hidden in the statistical noise on the data. Estimating the groundstate energy by fitting a straight line through the data points yields $E_{MC}/JL^2 = -2.21 \pm 0.01$ which is well within the bounds $-2.25 \leqq E_0/JL^2 \leqq -2.18$ [39].

Table 2. Energy per site of a 8×8 two-dimensional spin-1/2 XY model as a function of temperature. The statistical error have been determined by comparing different, independent runs

T	m	E_m
0.5	32	-2.142 ± 0.007
1.0	16	-2.138 ± 0.008
1.1	16	-2.119 ± 0.004
1.2	16	-2.104 ± 0.005
1.3	16	-2.093 ± 0.005
1.4	16	-2.070 ± 0.002
1.5	16	-2.043 ± 0.001

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